Repulsion and attraction in high Tc superconductors

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(Dated: January 4, 2011)

The influence of repulsion and attraction in high-Tc superconductors to the gap functions is studied. A systematic method is proposed to compute the gap functions using the irreducible representations of the point group. It is found that a pure s-wave superconductivity exists only at very low temperatures, and attractive potentials on the near shells significantly expand the gap functions and increase significantly the critical temperature of superconductivity. A strong on-site repulsion drives the A_{1g} gap into a B_{1g} gap. It is expected that superconductivity with the A_{1g} symmetry reaches a high critical temperature due to the cooperation of the on-site and the next-nearest neighbor attractions.

PACS numbers: 74.20.-z

I. INTRODUCTION

A few decades of study on high-Tc superconductor confirmed the $d_{x^2-y^2}$-wave symmetry of the gap function at least in cuprate superconductors, relative to the conventional s-wave gap symmetry[1, 2]. The newly discovered iron-based superconductors have a different gap symmetry from cuprates, expressed as $\sim \cos k_x \cos k_y$[3, 4], named as $s^{\pm}$-wave. Gap symmetries are believed to be results of point group symmetries of the superconductor crystals. Tsuei and Kirtley provided a systematic description to the gap symmetries from the point group theory[5]. The relation between the gap symmetries and the interaction, however, are not clear in literatures. That is to say, what interaction determines a given gap symmetry is still unknown.

The interaction in high-Tc superconductors is much more complicated than that in conventional s-wave superconductors. It is widely believed that the on-site repulsion of strongly correlated electrons drives Cooper pairs from s-wave to d-wave coupling. Monthous *et al*[6] gave a schematic picture for the interaction in cuprate superconductors as shown in Fig.1, where an electron locates at the center and another one hopping on the lattice. Due to the spin fluctuation repulsive potentials and attractive ones appear alternatively on the lattice sites but decay with increasing distances. A question is how they affect the gap functions of different symmetries and the critical temperatures of superconductivity. Understanding this mechanism may help humans design new superconductors with higher critical temperatures.

In this paper we first reveal the relation between the gap symmetries of a square lattice and the interactions on the lattice. This will provide a simple method for computing the gap functions of various symmetries. Using this method we analyze the influence of the repulsive and attractive potentials on neighboring sites to the gap functions and critical temperatures of superconductivity. Finally we conclude that superconductivity with the A_{1g} or B_{1g} gap symmetry may have much higher critical temperature than other symmetries, and an on-site attraction favors a A_{1g} gap symmetry but an on-site repulsion favors B_{1g}.

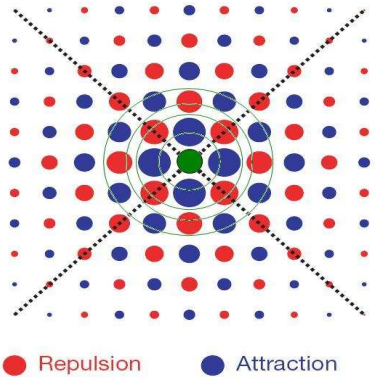

FIG. 1: Potentials between a quasi-particle at the center of a square lattice (green spot) and another one moving on the lattice (red or blue spots). The radii of the spots represent the strength of the potentials[6]. Each of the four light green circles connects the neighbors on a shell. From inner to outer the shells are labeled as I, II, II, and IV.

II. GAP FUNCTION

The BCS-type pairing Hamiltonian of superconductivity is written as

$$H_{pair} = \frac{1}{N}\sum_{kk'} V(\mathbf{k}'-\mathbf{k}) c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} c_{-k'\downarrow} c_{k'\uparrow} \qquad (1)$$

where $c^{\dagger}_{k\sigma}, c_{k\sigma}, \sigma = \uparrow, \downarrow$ are the creation and destruction operators of electrons with spin up and down. Note that a factor $1/N$ has been added in the Hamiltonian. It is

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necessary for convergence over k-space summation but missing in literatures for decades. The potential $V(\mathbf{q})$ is expanded into the real space

$$V(\mathbf{q}) = (1/2)\sum_{\mathbf{m}} V(\mathbf{m})e^{-i\mathbf{q}\cdot\mathbf{m}} \tag{2}$$

where $V(\mathbf{m})$ is the potential energy between an electron at the center and another one at site $\mathbf{m}$, as shown in Fig.1.

The central site has the first shell neighbors, i.e., the nearest neighbors($n.n.$), the second shell neighbors, i.e., the next nearest neighbors($n.n.n.$), the third shell ones, and the fourth shell ones, etc. In general, only the on-site potential and the potentials on the four near shells, $V_L, L = 0, 1, 2, 3, 4$, are important. Therefore, these five parameters determine the pairing Hamiltonian thus the properties of superconductivity. The gap function is given by the following well-known gap equation[7]

$$\Delta_{\mathbf{k}} = -\frac{1}{N}\sum_{\mathbf{k}'} V(\mathbf{k}-\mathbf{k}')\frac{\tanh(\xi_{\mathbf{k}'}/2kT)}{2\xi_{\mathbf{k}'}}\Delta_{\mathbf{k}'} \tag{3}$$

where $\xi_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$ is the energy of a quasi-particle, and $\epsilon_{\mathbf{k}}$ is the free-electron energy on a square lattice given by $\epsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$. Changing the above gap function from k-space into the real space using a Fourier transformation $\Delta_{\mathbf{k}} = \sum_{\mathbf{m}} \Delta(\mathbf{m})e^{-i\mathbf{k}\cdot\mathbf{m}}$ one obtains

$$\Delta(\mathbf{m}) = -\frac{V(\mathbf{m})}{2N}\sum_{\mathbf{m}',\mathbf{k}'} \frac{\tanh(\xi_{\mathbf{k}'}/2kT)}{2\xi_{\mathbf{k}'}} e^{i\mathbf{k}'\cdot(\mathbf{m}-\mathbf{m}')}\Delta(\mathbf{m}') \tag{4}$$

Compared to the case of k-space the above equation has much smaller dimensions, which is in general smaller than 21×21 as defined by the 20 neighbors of the four shells around the central one in Fig.1. The dimensions can be further reduced up to 5×5 when lattice symmetries are included. In particular, obviously, a unique on-site potential V_0 will result in a k-independent potential $V(\mathbf{k}) = V_0$ thus the conventional s-wave constant gap function $\Delta(0)$. Dominant neighboring potentials V_1, V_2, V_3, V_4 lead to the unconventional superconductivity, such as the d-wave ones.

III. THE SYMMETRIES OF GAP FUNCTIONS ON A SQUARE LATTICE

The gap equation (4) is symmetric about the point group G of the lattice since $\epsilon_{Rk} = \epsilon_k, V(R\mathbf{m}) = V(\mathbf{m}), R \in G$, that is

$$\Delta(R\mathbf{m}) = -\frac{V(\mathbf{m})}{2N}\sum_{\mathbf{m}',\mathbf{k}'} \frac{\tanh(\xi_{\mathbf{k}'}/2kT)}{2\xi_{\mathbf{k}'}} e^{i\mathbf{k}'\cdot(\mathbf{m}-\mathbf{m}')}\Delta(R\mathbf{m}') \tag{5}$$

This shows that the gaps $\Delta(\mathbf{m})$ transform according to the irreducible representations (IR's) of the point group G, i.e.,

$$\Delta^{(j)}(R\mathbf{m}) = \sum_i T_{ij}^{\alpha}(R^{-1})\Delta^{(i)}(\mathbf{m}) \tag{6}$$

where $T^{\alpha}(R^{-1})$ is the matrix of IR α for group element R^{-1}. It is seen that gaps $\Delta(\mathbf{m})$ on the same shell differ from each other at most by a matrix $T^{\alpha}(R^{-1})$. In particular, they differ only by a phase factor for one dimensional IR's. This property is represented by the basis functions of IR's, i.e., gaps $\Delta(\mathbf{m})$ transform under the point group just as the basis functions do.

A 2D square lattice has a point group symmetry of D_4. This group has five IR's $A_{1g}, A_{2g}, B_{1g}, B_{2g}$ and Eg and their corresponding basis functions as listed in Table I.

Table I. Irreducible representations and basis functions.

IR	Basis function	Allowed shells	Wave type
A_{1g}	$1, (x^2+y^2)/2$	0,I-IV	$s + s^{\pm}$
A_{2g}	$xy(x^2-y^2)/2$	IV	g
B_{1g}	$(x^2-y^2)/2$	I, III, IV	$d_{x^2-y^2}$
B_{2g}	xy	II,IV	d_{xy}
Eg	$\binom{x+iy}{x-iy}$	I-IV	p

The first four of these IR's are one dimensional and the last one is two dimensional. The basis functions of the five IR's listed in Table I vanish except on the allowed shells. For example, a g-wave can only occur on shell IV, and a d_{xy}-wave on shells II and IV, *etc.* Then gaps $\Delta(\mathbf{m})$ are given by

$$\Delta(\mathbf{m}) = \frac{f_{IR}(x_m, y_m)}{|f_{IR}(x_m, y_m)|}\Delta_{L_{\mathbf{m}}}, \quad \mathbf{m} \neq 0 \tag{7}$$

where $f_{IR}(x_m, y_m)$ is the value of the basis function at site (x_m, y_m), and $\Delta_{L_{\mathbf{m}}}$ is the magnitude of $\Delta(\mathbf{m})$ on shell L_m.

Using (7) and making an inverse Fourier transformation to $\Delta(\mathbf{m})$ one obtains the gap functions of every IR,

$$\begin{aligned}\Delta_{A_{1g}}(\mathbf{k}) &= \Delta_0 + 2\Delta_1(\cos k_x + \cos k_y) \\ &\quad + 4\Delta_2 \cos k_x \cos k_y + 2\Delta_3(\cos 2k_x + \cos 2k_y) \\ &\quad + 4\Delta_4(\cos 2k_x \cos k_y + \cos k_x \cos 2k_y) \end{aligned} \tag{8}$$

$$\Delta_{A_{2g}}(\mathbf{k}) = 4\Delta_4(\sin k_x \sin 2k_y - \sin 2k_x \sin k_y) \tag{9}$$

$$\begin{aligned}\Delta_{B_{1g}}(\mathbf{k}) &= 2\Delta_1(\cos k_x - \cos k_y) \\ &\quad + 2\Delta_3(\cos 2k_x - \cos 2k_y) \\ &\quad + 4\Delta_4(\cos 2k_x \cos k_y - \cos k_x \cos 2k_y) \end{aligned} \tag{10}$$

$$\begin{aligned}\Delta_{B_{2g}}(\mathbf{k}) &= -4\Delta_2 \sin k_x \sin k_y \\ &\quad - 4\Delta_4(\sin 2k_x \sin k_y + \sin k_x \sin 2k_y) \end{aligned} \tag{11}$$

$$\Delta_{E_g}(\mathbf{k}) = -2\Delta_1(iu\sin k_x - v\sin k_y) - 4\Delta_2(iu\sin k_x\cos k_y - v\cos k_x\sin k_y) - 4\Delta_3(iu\sin 2k_x - v\sin 2k_y) - 4\Delta_4[iu(\sin k_x\cos 2k_y + 2\sin 2k_x\cos k_y) - v(\cos 2k_x\sin k_y + 2\cos k_x\sin 2k_y)] \quad (12)$$

where $\Delta_L, L = 0,1,2,3,4$ are the magnitudes of the on-site gap and the gaps on the four shells, and $u = \frac{1}{\sqrt{2}}\binom{1}{1}, v = \frac{1}{\sqrt{2}}\binom{1}{-1}$. A s-wave gap Δ_0 has been added into the gap function of A_{1g} since the basis function of this IR is circularly symmetric. That is to say, a s-wave gap coexists only with that of the A_{1g} symmetry. Which gap symmetry is selected by a superconductor is determined by the lowest condensation energy of the system.

These gap functions are simpler and clearer than the earlier results obtained by Tsuei and Kirtley[5]. They gave only the first terms of these gap functions. We will see in the next section that the first terms may not be dominant. It should be emphasized that in general gap functions of different symmetries do not mix together, unless the symmetry (5) is broken. Mixing gap functions were considered due to minor anisotropy in the a and b directions on CuO_2 planes, such as $d_{x^2-y^2} + id_{xy}$ proposed by Ghosh *et al*[8] and $s + d_{x^2-y^2}$ by Müller *et al*[9–11].

IV. CRITICAL TEMPERATURES

The gap functions of different symmetries are easily worked out through self-consistent computations to (4) given potential energies V_L on different shells of a square lattice. It is found that the critical temperatures of superconductivity of different gap symmetries are significantly different.

In Fig.2, a pure s-wave gap is created by a pure on-site attractive potential $V_0 = -0.5$ and gaps with the A_{1g} symmetry are created by the same on-site potential and other four $-0.1, -0.2, -0.1, -0.01$ on the four near shells. It is seen that the s-wave gap exists only below a very low temperature of about $0.00018t$. Small attractive potentials on the near shells, especially on shell II, extends the on-site gap a few times and increases the critical temperature more than five times. Therefore, superconductivity is significantly enhanced by a pairing on the $n.n.n.$ with the A_{1g} symmetry. This pairing has two main components Δ_0 and Δ_2. This leads to a mixing $s + s^{\pm}$ gap function $\Delta(\mathbf{k}) \approx \Delta_0 + \Delta_2\cos k_x\cos k_y$. It has different signs at the center and $(\pi, 0)$ of the BZ just as the case in iron pnictides[12]. Further computations show that the potential on shell I, V_1, even if strongly repulsive, e.g. 0.4, does not influence $\Delta(\mathbf{k})$ significantly. This is similar to the result obtained by Wang and co-workers[13] for iron pnictides. This form of gap function is much more robust than the widely assumed form $\cos k_x + \cos k_y$ in literatures[14].

When the attractive potential on shell II, V_2, increases

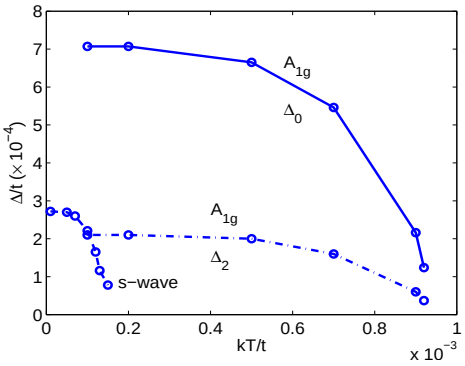

FIG. 2: Comparison between the gap of a pure s-wave and those of the A_{1g} symmetry. The pure s-wave gap is created by a pure, on-site, attractive potential $V_0 = -0.5$, and the gaps of A_{1g} by the five potentials $V_L = -0.5, -0.1, -0.2, -0.1, -0.01$. Band parameters are set to be $t = 1.0, t' = -0.125, \mu = -0.527$ for a hole concentration of 0.125.

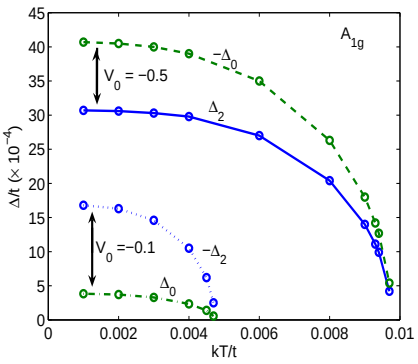

FIG. 3: Gaps with on-site potentials -0.1 and -0.5. The four-shell potentials are $-0.1, -0.5, -0.2, -0.01$. Band parameters are $t = 1.0, t' = -0.125, \mu = -0.527$.

to -0.5 the gaps dramatically expand as shown in Fig.3. Under the cooperation of attractive V_0 and V_2 the gaps increase significantly leading to a dramatic increase of T_c (about 52 times compared to the pure s-wave case). If the on-site attraction is weak the gap is mainly of a $s^{\pm}$ wave. Thus the superconductivity is significantly enhanced by the shell II pairing with the A_{1g} symmetry. This provides a possibility for researchers to increase the T_c of superconductivity by means of increasing the attraction on shell II atoms. This is just the case of the iron-based superconductors. It is expected that these superconductors may have much higher critical temperatures than other series of superconductors.

In cuprates, however, there is a strong on-site Coulombic repulsion due to the strong correlation effect. Thus a on-site pairing is energetically expensive in these superconductors. The gaps with the A_1 and B_1 symmetries under different on-site potentials are shown in Fig.4. It is seen that the on-site repulsion strongly reduces the gaps with the A_{1g} symmetry but holds those with the B_{1g}

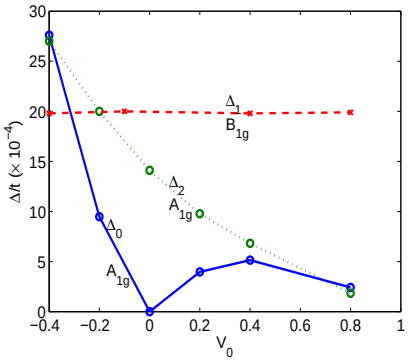

FIG. 4: Gaps under different on-site potentials V_0. Potentials on the four shells are $-0.3, -0.5, -0.2, -0.01$. $t = 1.0, t' = -0.125, \mu = -0.527$.

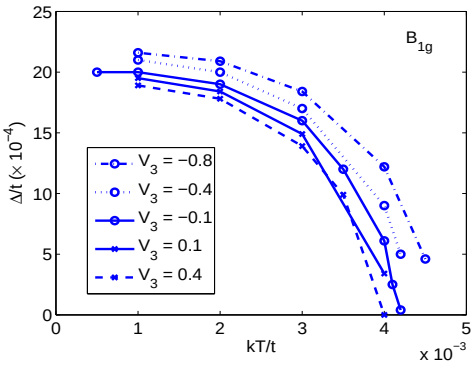

FIG. 5: Gap Δ_1 with the B_{1g} symmetry vs potential on shell III. Other potentials are $-0.1, -0.5, -0.2, -0.01$ except V_3. $t = 1.0, t' = -0.125, \mu = -0.527$

symmetry. Therefore, under a strong on-site repulsion a pairing with the B_{1g} symmetry, i.e. a $d_{x^2-y^2}$ wave, is much more energetically favorable. This is just the case in cuprates which display a d-wave superconductivity.

A question is whether this B_{1g} pairing can be further enhanced by increasing attractive potentials on other shells. It is found through computations that the potential on shell II, no matter attractive or repulsive, does not affect the B_{1g} pairing, but V_3 has a weak influence to the gap, as shown in Fig.5. Δ_1 increases only slightly with more attractive V_3 but even a repulsive V_3 does not break the B_{1g} pairing.

Gaps with other symmetries A_{2g}, B_{2g} and E_g are verified through computations to be small and result in low critical temperatures. Superconductivity with the A_{1g} and B_{1g} symmetries is most expectable to go into the higher temperature region.

V. CONCLUSION

In this work we studied the influence of repulsion and attraction in high temperature superconductors to the gap functions and transition temperatures. We proposed a systematic method to compute the gap functions using the irreducible representations of the crystalline point group. Then we analyze the gap functions with various symmetries for different potential energies at different temperatures. It is found that a pure s-wave superconductivity exists only at very low temperatures, and attractive potentials on the near shells significantly expand the gap functions and increase dramatically the critical temperatures. Especially the A_{1g} gap is expanded by an on-site attractive potential and that on the next nearest neighbors, thus increases the critical temperature for tens of times. A strong on-site repulsion, however, blows up the A_{1g} gap but keeps a B_{1g} gap survive. It is expected that superconductivity with the A_{1g} symmetry has a high critical temperature.

This work was supported by the National Natural Science Foundation of China (Grant No. 10874049), the State Key Program for Basic Research of China (No. 2007CB925204) and the Natural Science Foundation of Guangdong province (No. 07005834).

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